Fenarimol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 129 °C

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 5.95e-01

Nearest Neighbors from the Training Set

Image not found
Fenarimol
Measured: 118
Predicted: 129

Image not found
Nuarimol
Measured: 126
Predicted: 132

Image not found
Bromperidol
Measured: 155
Predicted: 149

Image not found
Haloperidol
Measured: 152
Predicted: 148